

# Quantum Scattering in Strong Cylindrical Confinement

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## Abstract

A Green's function formalism to analyze the scattering properties in confined geometries is developed. This includes scattering from a central field inside the guide created e.g. by impurities. For atomic collisions our approach applies to the case of parabolic confinement and, with certain restrictions, also to an anharmonic one. The coupling between the angular momentum phase shifts  $\delta_l$  of a spherically symmetric scattering potential  $V(r)$  due to the cylindrical confinement is analysed. Under these general conditions, a broad range of scattering energies covering many transversal excitations is considered and changes to the bound states of  $V(r)$  are derived. For collisions between identical atoms, the boson-fermion and fermion-boson mappings are demonstrated.

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Implementing atom-optical devices often requires a strong confinement for all except one degree of freedom [1, and Refs therein]. Examples of physical situations where a strong confinement is needed are guided matter-wave interferometers [1], one dimensional optical lattices [2], cold gases in very elongated traps for studies of superfluidity [3], the Tonks-Girardeau gas [4] or phase fluctuations of quasi-condensates [5]. A proper description of the dynamics of such reduced quasi-1D systems should account for the nature of the discrete transverse states. Therefore one needs to deduce the effective 1D interaction between the remaining longitudinal degrees of freedom from the real 3D free-space interaction potential  $V(r)$ . Collisions under confinement different from the 1D case are treated in [6, 7]. Apart from ultracold *atom-atom collisions*, scattering in confined geometries also occurs in various physical situations such as scattering of guided atomic matter waves or of guided electromagnetic and acoustic waves [8] from *obstacles inside a guide*, e.g., (heavy) impurity atoms or material defects, respectively. The latter is of importance for the propagation of radiation or sound within transmission lines or resonators.

As for atom-atom collisions, resonant quasi-1D scattering in the transverse ground state of the guide (single mode regime) was first considered for bosons in an harmonic guide employing for the interaction potential  $V(r)$  a delta-like zero-range approximation [9]. Numerical simulations [10] confirmed for certain finite range potentials  $V(r)$  the existence of the so-called confinement induced resonance (CIR) originally predicted in [9]. A further investigation of the CIR is provided in [11] dealing for the first time with a general finite-range  $V(r)$  for both bosons and fermions under harmonic confinement. Effects of the non-parabolicity of the confinement are considered in [12], with focus on the center of mass dynamics and employing a zero-range approximation for the interaction  $V(r)$ .

The present work extends the above approaches and gives an alternative and complementary description of scattering under confinement, treating both the cases of collisions and of scattering by fixed obstacles. We develop a general formalism based on the Green's functions that allows us to express the scattering properties in confined geometries in terms of the phase-shifts  $\delta_l$  of free-space scattering. The coupling between these phase-shifts is explicitly taken into account. A general initial scattering state can be treated properly, describing in particular the “multi-channel” regime, in the sense that the total energy allows several transversal excited states to be effectively occupied.

In the case of collisions where  $V(r)$  is the atom-atom interaction potential, the center of

mass motion is known to separate from the relative one only for a *parabolic confinement*. Our approach then provides a deeper understanding of this collision process. On the other hand, for an *arbitrary confinement*, scattering processes that can naturally be described by the formalism include, e.g., the quantum scattering of individual cold atoms, or other equivalent systems, by a central field  $V(r)$  fixed in the center of the guide at  $\mathbf{r} = 0$ . As for atom-atom scattering, the relative coordinates  $\mathbf{r}$  are not exactly separable from the center of mass coordinates  $\mathbf{R}$  if the confinement is no longer parabolic. Nevertheless, in such a situation of coupled center of mass and relative motion, the formalism provides in the ultracold regime a distinct starting-point to account for this coupling.

Under the above restrictions concerning atom-atom collisions, our investigation confirms that the CIR [9] is a general consequence of the dominant terms of the scattering amplitudes. The main requirements are a large positive  $s$ -wave scattering length  $a$ ,  $a \sim l_\perp$  [ $l_\perp$  is the length scale of the confining potential  $U(\rho)$ , such that  $U \approx 0$  for  $\rho \ll l_\perp$ , and equals the cylinder radius for a square-well type confinement], a short-ranged scattering potential  $V(r)$ ,  $R_V \ll l_\perp$  [ $R_V$  is the range of  $V(r)$ , such that  $V \approx 0$  for  $r \gg R_V$ ], small longitudinal momenta and small phase-shifts  $\delta_l$ , as described below. The resonance is accompanied by a  $l = 0$  bound-state of  $V(r)$  strongly distorted by the confinement  $U(\rho)$  and pushed towards the continuum. This modified bound state [10] is shown to be a herald of the CIR. In the context of scattering of individual guided atoms by a central field, these conclusions hold irrespective of restrictions due to anharmonicities and imply the unambiguous strong effects of confinement on the scattering process.

*Phase-Shifts.* The Schrödinger equation for the scattering wave function  $\Psi(\mathbf{r})$ , with  $\mathbf{r} = (\boldsymbol{\rho}, z)$ , reads

$$[\nabla^2 - u(\rho) + k^2] \Psi(\mathbf{r}) = v(r)\Psi(\mathbf{r}), \quad (1)$$

where  $u(\rho) \equiv 2\mu U(\rho)/\hbar^2$ ,  $v(r) \equiv 2\mu V(r)/\hbar^2$ , and  $E = \hbar^2 k^2/2\mu > 0$  is the total energy. In the case of atomic collisions,  $\mathbf{r}$  is the relative coordinate and the relation between  $U(\rho)$  and the confining potential  $U_c(\rho_i)$  of the  $i$ -th particle in the laboratory reference frame is given by  $U(\rho) = 2U_c(\rho/2)$ . Note that this relation is no longer exact for non-parabolic  $U_c$  (but provides a first uncoupled description of the relative motion, by quenching the center of mass at the origin  $\mathbf{R} = 0$ ). The cylindrical boundary condition is met by expanding the solution in the transverse eigenstates  $\varphi_n(\rho)$ , with energies  $\epsilon_n \equiv \hbar^2 q_n^2/2\mu$  and normalized to

$\int dx dy \varphi_n(\rho)^* \varphi_m(\rho) = \delta_{nm}$ . As a result, one obtains the integral equation

$$\Psi(\mathbf{r}) = \Psi_i(\mathbf{r}) - \int d^3 \mathbf{r}' G_c(\mathbf{r}, \mathbf{r}') v(\mathbf{r}') \Psi(\mathbf{r}'). \quad (2)$$

For a given  $k$  low enough such that  $k \sim 1/l_\perp$ , let  $n_E$  be the integer obeying  $k^2 = q_{n_E}^2 + k_{n_E}^2 \leq q_{1+n_E}^2$ . The following study includes the situations of ground state scattering ( $n_E = 0$ ) as well as scattering in the *transversally excited* modes ( $n_E \geq 1$ ). In both cases, transverse states with  $n > n_E$  can only be *virtually* occupied, since  $k^2 < q_n^2$ . The general initial state is  $\Psi_i(\mathbf{r}) = \sum_{n=0}^{n_E} b_n e^{ik_n z} \varphi_n(\rho)$  for some constants  $b_n$ , with  $k^2 = q_n^2 + k_n^2$ . In Eq.(2),

$$G_c(\mathbf{r}, \mathbf{r}') = \sum_{n=0}^{\infty} \varphi_n(\rho) \varphi_n(\rho')^* G_n(z - z') \quad (3)$$

is an axially symmetric Green's function and  $G_n(z) = -e^{ik_n |z|} / 2ik_n$  (for  $n \leq n_E$ ) and  $G_n(z) = e^{-p_n |z|} / 2p_n$  (with  $k^2 = q_n^2 - p_n^2$ , for  $n \geq 1 + n_E$ ) are 1D Green's functions. The excited states with quantum numbers larger than  $n_E$  decrease exponentially with increasing distance from the scattering region. In the asymptotic limit  $|z| \rightarrow \infty$ , one has for  $n \leq n_E$

$$\Psi(\mathbf{r}) \approx \sum_{n=0}^{n_E} [b_n e^{ik_n z} + f_n^\pm e^{ik_n |z|}] \varphi_n(\rho), \quad z \rightarrow \pm\infty, \quad (4a)$$

$$f_n^\pm \equiv \frac{1}{2ik_n} \int d\mathbf{r}' [e^{\pm ik_n z'} \varphi_n(\rho')]^* v(\mathbf{r}') \Psi(\mathbf{r}'), \quad (4b)$$

where  $f_n^\pm$  is the  $n$ -th channel *effective 1D scattering amplitude* for forward  $z > 0$  and backward  $z < 0$  scattering.

Consider next  $G_c(\mathbf{r}, \mathbf{r}')$  for  $r' < r \ll l_\perp$ . In this region  $U(\rho) \approx 0$  and one should be able to approximate  $G_c$  by the free 3D Green's functions  $G_{1,2}(\mathbf{r}, \mathbf{r}') \equiv e^{\pm ik|\mathbf{r}-\mathbf{r}'|} / 4\pi|\mathbf{r}-\mathbf{r}'|$ . Thus, we write

$$G_c(\mathbf{r}, \mathbf{r}') = \frac{1}{2\pi} \int d\phi' \left( \gamma_+ \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} + \gamma_- \frac{e^{-ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} \right) + \Delta_c(\mathbf{r}, \mathbf{r}') \quad (5a)$$

$$= ik \sum_l j_l(kr') \left[ \gamma_+ h_l^{(1)}(kr) - \gamma_- h_l^{(2)}(kr) \right] \times \frac{2l+1}{4\pi} P_l(\cos \theta) P_l(\cos \theta') + \Delta_c(\mathbf{r}, \mathbf{r}'), \quad r' < r \ll l_\perp. \quad (5b)$$

In Eq.(5b), we have used the well known expansion of  $G_{1,2}$  in spherical coordinates [13, Prob.7.5]. The value of  $\gamma_\pm$  and  $\Delta_c$  can be explicitly obtained if  $U(\rho)$  is approximated by a

*square-well* type confinement for  $r \ll l_\perp$ . Indeed, the eigenstates are then close to Bessel functions,  $\varphi_n(\rho) \approx N_n J_0(q_n \rho) / \pi^{1/2} l_\perp$ , normalized on a disc of radius  $l_\perp$ ,  $N_n = 1/|J_1(r_{n+1})|$ ,  $r_{n+1}$  being the  $(n+1)$ -th root of  $J_0$ . Separating from  $G_c$  the terms  $n \leq n_E$ , the series for  $n > n_E$  can be approximated by an integral over  $q$  emerging from the continuum limit  $q_n \rightarrow q$  and valid when  $r', r \ll l_\perp$ . Note that  $q$  starts at  $q_{1+n_E} > k$ . One then compares real and imaginary parts of  $G_c$  in Eq(3) with a suitable expansion of  $G_{1,2}$  in *cylindrical* coordinates [13, Prob.7.9] in Eq(5a). This comparison leads to

$$\gamma_\pm = 1/2 \pm \gamma/2, \quad \gamma \equiv \sum_{n=0}^{n_E} 2N_n^2 / k k_n l_\perp^2, \quad (6a)$$

$$\Delta_c(\mathbf{r}, \mathbf{r}') \equiv -\frac{1}{4\pi} \int_0^{p_c} dp e^{-p|z-z'|} J_0(q\rho) J_0(q\rho'), \quad (6b)$$

with  $q = \sqrt{k^2 + p^2}$  and  $q_{1+n_E} \equiv \sqrt{k^2 + p_c^2}$ . The homogeneous (Helmholtz) term  $\Delta_c$  corrects the Green's function  $\gamma_+ G_1 + \gamma_- G_2$ , with  $\gamma_+ + \gamma_- = 1$ , in order to account for the discreteness due to the confinement. Within the flatness condition, the above approach is valid for arbitrary  $U(\rho)$ . It yields an intrinsic connection between the confined and the free space scattering approaches (see [9] for parabolic confinement).

In order to obtain the scattering phases  $\delta_l$  that are associated with the spherical symmetry, we expand the incident state in spherical coordinates employing  $e^{ik_n z} \varphi_n(\rho) = \sum_l i^l (2l+1) \alpha_{nl} j_l(kr) P_l(\cos \theta)$ , with  $\alpha_{nl} = N_n P_l(k_n/k) / \pi^{1/2} l_\perp$  [13]. Analogously in  $\Delta_c$ , the equivalent expansion is given by  $e^{-pz} J_0(q\rho) = \sum_l i^l (2l+1) P_l(ip/k) j_l(kr) P_l(\cos \theta)$  stemming from an analytic continuation into the complex  $\theta$ -plane ( $\theta \rightarrow \pi/2 - i\theta$ ). Inserting these expressions and Eq.(5b) into Eq.(2) and using Eq.(6a) yields, for  $R_V \ll r \ll l_\perp$ ,

$$\begin{aligned} \Psi(\mathbf{r}) \approx & \sum_l i^l (2l+1) [\alpha_l + \gamma_l(z) - i\gamma k T_l] j_l(kr) P_l(\cos \theta) \\ & + \sum_l i^l (2l+1) [k T_l] n_l(kr) P_l(\cos \theta), \end{aligned} \quad (7)$$

with  $\alpha_l = \sum_{n=0}^{n_E} b_n \alpha_{nl}$ . Here  $4\pi T_l \equiv i^{-l} \int d^3 \mathbf{r}' [j_l(kr') P_l(\cos \theta')] v(r') \Psi(\mathbf{r}')$  and  $4\pi \gamma_l(z) \equiv \int_0^{p_c} dp \int_{(z)} d^3 \mathbf{r}' P_l(\pm ip/k) e^{\pm pz'} J_0(q\rho') v(r') \Psi(\mathbf{r}')$ . The integration over  $\mathbf{r}'$  for  $\gamma_l(z)$  is performed in a finite volume  $\Omega$  covering the range of  $v(r')$ . If  $z$  is outside  $\Omega$ , the positive sign refers to a positive  $z$  and vice-versa. Inside  $\Omega$ , both signs are needed according to whether  $z \gtrless z'$ . Except for this  $z$ -dependence of  $\gamma_l(z)$  in Eq.(7), we have now succeeded in representing the total scattering wave function in spherical coordinates.

Noteworthy at this point is the fact that  $\gamma_l(z)$  accounts for *couplings* between different angular momenta. Indeed, by using  $e^{\pm pz'} J_0(q\rho') = \sum_{l'} i^{l'} (2l' + 1) P_{l'}(\mp ip/k) j_{l'}(kr') P_{l'}(\cos \theta')$  and the property  $P_{l'}(\mp u) = (-1)^{l'} P_{l'}(\pm u)$  in the definition of  $\gamma_l(z)$ , one gets a constant  $\gamma_l(z)$  if, for each  $l$ , only  $l'$ -waves are kept such that  $l + l' = \text{even}$ . The latter condition is also necessary to obtain non-zero matrix elements  $\langle l | U(\rho) | l' \rangle$  due to the parity symmetry  $\mathbf{r} \rightarrow -\mathbf{r}$ . Therefore, a constant  $\gamma_l(z) \approx \gamma_l$  arises

$$\gamma_l = \sum_{l' [l]} (2l' + 1) P_{l'} T_{l'}, \quad l = 0, 1, 2, \dots, \quad (8)$$

where  $P_{l'} \equiv k \int_0^{p_c/k} du P_l(iu) P_{l'}(iu)$  and  $l' [l]$  denotes the sum over even (odd)  $l'$  for even (odd)  $l$ . Eq.(8) is equivalent to the condition that the “perturbation”  $U(\rho)$  to the free space scattering does not couple even and odd angular momenta.

It is now possible to introduce the phase-shifts  $\delta_l$ . The solution Eq.(7) can be written as ( $R_V \ll r \ll l_\perp$ )

$$\Psi(\mathbf{r}) \approx \sum_l c'_l [\cos \delta_l j_l(kr) - \sin \delta_l n_l(kr)] P_l(\cos \theta), \quad (9a)$$

$$c'_l \equiv \frac{(2l + 1)(\alpha_l + \gamma_l) i^l}{\cos \delta_l - i\gamma \sin \delta_l}, \quad T_l \equiv \frac{\alpha_l + \gamma_l}{i\gamma k - k \cot \delta_l}, \quad (9b)$$

where the last two relations *define* formally  $c'_l$  and  $\delta_l$ . That this  $\delta_l$  is the actual phase-shift can be seen as follows. On one hand, Eq.(9a) is the (intermediate) asymptotics  $R_V \ll r \ll l_\perp$  of the solution  $\Psi(\mathbf{r}) = \sum_l c'_l R_l(r) P_l(\cos \theta)$  in the region of  $V(r)$ . On the other hand, the free-space scattering solution in this region, i.e., not taking into account the boundary, is just a *different superposition*  $\Psi_{3D}(\mathbf{r}) = \sum_l c_l R_l P_l$  with the *same* radial part  $R_l$ . In other words, the effect of the confinement  $U(\rho)$  is to change the superposition coefficients from  $c_l$  to  $c'_l$  while keeping the scattering phases of the free-scattering problem. Then the second relation in Eq.(9b) together with Eq.(8) gives a *matrix equation* for  $T_l$  in terms of  $\delta_l$ , i.e., for  $l = 0, 1, 2, \dots$

$$(i\gamma k - k \cot \delta_l) T_l = \alpha_l + \sum_{l' [l]} (2l' + 1) P_{l'} T_{l'}. \quad (10a)$$

Finally, the effective amplitude  $f_n^\pm$  is given by expanding  $e^{\pm i k_n z'} \varphi_n(\rho')$  in the integrand of Eq.(4b), thus

$$f_n^\pm = f_{ng} \pm f_{nu} \equiv \left( \sum_{l \text{ even}} \pm \sum_{l \text{ odd}} \right) \frac{(2l + 1) 4\pi \alpha_{nl}}{2i k_n} T_l. \quad (10b)$$

The relationship between the amplitudes in Eq.(10b) and the matrix elements  $T_l$  of Eq.(10a) constitutes the main result of our formalism.

*Current Conservation.* Inserting Eqs.(10a,10b) into Eq.(4), the probability conservation should follow. From the total current along the  $z$ -axis, the conservation condition is

$$0 = \sum_{n=0}^{n_E} (|f_{ng}|^2 + \text{Re}\{b_n^* f_{ng}\} + |f_{nu}|^2 + \text{Re}\{b_n^* f_{nu}\}) k_n. \quad (10c)$$

In the remainder of this paper, we analyse the scattering process given by the leading terms of Eqs.(10). We consider first the case of the single mode regime in more detail, followed by the case of transverse excitations and angular momenta couplings.

*Single Mode Resonances.* When only the ground state ( $n_E = 0$ ,  $b_n = \delta_{0n}$ ,  $k^2 = q_0^2 + k_0^2$ ) represents an open channel, the symmetric and antisymmetric sectors of Eq.(4a),  $\Psi(\mathbf{r}) = [\psi_g(z) + \psi_u(z)] \varphi_0(\rho)$ , are given respectively by (for  $z \gtrless 0$ )

$$\psi_g(z) = (1 + f_{0g}) \cos(k_0 z) + i f_{0g} \sin(k_0 |z|), \quad (11a)$$

$$\psi_u(z) = i(1 + f_{0u}) \sin(k_0 z) \pm f_{0u} \cos(k_0 z). \quad (11b)$$

In the context of collisions between identical particles, it is clearly seen that, at resonance  $f_{0g} = -1$ , the bosonic sector  $\psi_g$  is mapped into a non-interacting  $f_{0u} = 0$  pair of (spin-polarized) fermions, the well known fermionization of impenetrable bosons. Now, the inverse is also seen to occur for  $\psi_u$  at the fermionic resonance,  $f_{0u} = -1$ , first obtained in [11]. A further insight is gained by setting

$$f_{0g,u} = -[1 + i \cot \delta_{g,u}]^{-1}. \quad (12)$$

The conservation condition Eq.(10c) is then fulfilled for real 1D phase-shifts  $\delta_{g,u}$  and one can rewrite  $\psi_g = e^{i\delta_g} \cos(k_0 |z| + \delta_g)$  and  $\psi_u = i e^{i\delta_u} \sin(k_0 z \pm \delta_u)$ . Thus at resonance  $|\delta_{g,u}| = \pi/2$  and the above discussed boson-fermion and fermion-boson mappings exist also under longitudinal confinement, e.g., by imposing  $\psi_{g,u}(z = l_{\parallel}) = 0$ , as numerically verified in Ref. [11].

*CIR and bound-states.* The resonance  $f_{0g} = -1$  can be calculated from a general potential  $V(r)$  by solving Eq.(10a) for even  $l$ . Since  $kR_V \sim R_V/l_{\perp} \ll 1$ , the phase-shifts  $\tan \delta_l = \tan \delta_l(k) \sim k^{2l+1} \sim 1/l_{\perp}^{2l+1}$  are generally small [14] for large  $l_{\perp}$ . From Eq.(10a), it follows that  $l = 0$  is the leading contribution and  $f_{0g}$  has the form compatible with Eq.(12)

$$f_0^{\pm} \approx f_{0g} \approx -\frac{1}{1 + i \left[ -\frac{d_{\perp}^2}{2a} (1 - aP_{00}) \right] k_0}, \quad (13a)$$

where  $d_\perp \equiv l_\perp/N_0$ ,  $P_{00} = p_c$ , and  $a$  is the 3D  $s$ -wave scattering length,  $k \cot \delta_0 \approx -1/a$ . This corresponds to solving for  $z$  under an effective 1D pseudopotential  $V_{1D}(z) = g_{1D}\delta(z)$ , with the coupling strength

$$g_{1D} = \frac{\hbar^2}{\mu} \frac{2a}{d_\perp^2} \left(1 - \frac{C'a}{d_\perp}\right)^{-1}, \quad C' \equiv d_\perp p_c. \quad (13b)$$

As in previous works in the single mode regime (for atom-atom collisions in parabolic confinement) [9, 10, 11], the resonance  $|g_{1D}| \rightarrow \infty$  at  $d_\perp \approx C'a$  requires low longitudinal momenta  $k_0 \ll k \sim 1/l_\perp$ , such that  $p_c \xrightarrow{k_0 \rightarrow 0} \sqrt{q_1^2 - q_0^2}$  is not negligible, and large positive scattering length  $0 < a \sim l_\perp$  (meaning that a weak bound-state of  $V(r)$  approaches the threshold [14]). For scattering by a central field, not only  $V(r)$  but also  $U(\rho)$  can be quite general.

Viewing CIR as a low energy resonant scattering, one could say that bound-states close to threshold are neither probed at “high” energies  $k_0 \sim 1/l_\perp$  ( $k \rightarrow q_1$ ,  $p_c \rightarrow 0$ ), nor do they exist for small scattering lengths ( $a \ll d_\perp$ ). However, by calculating the bound-state with energy  $E'_B$ , this interpretation for the physical mechanism behind CIR is not accurate:  $f_{0g} \approx -1$  occurs before  $E'_B$  approaches zero (threshold without confinement), whereas  $E'_B \rightarrow \epsilon_0$  (threshold under confinement) occurs only if  $l_\perp$  is decreased much further below its CIR value. This is explicitly verified e.g. when  $U(\rho)$  is a square-well box of radius  $l_\perp$ : using a cosine approximation to  $J_0$  for its roots,  $q_0 \approx 3\pi/4l_\perp$  and  $q_1 \approx 7\pi/4l_\perp$ , whence  $C' = d_\perp \sqrt{q_1^2 - q_0^2} = \sqrt{20/3} = 2.58$  (see [10] for parabolic  $U(\rho)$  and zero-range atom-atom interaction).

In fact, the outer  $l = 0$  bound-state of  $V(r)$  in the absence of the confinement has the energy  $E_B \equiv -\hbar^2 \kappa_B^2 / 2\mu$  that is related to  $a$  via  $\kappa_B \approx 1/|a|$ , when  $a \gg R_V$  [14]. Under lateral confinement, its tail  $e^{-\kappa_B r}$  is changed to be zero at the edge  $r = \rho = l_\perp$ . By the uncertainty principle, this slight squeeze lifts  $E_B < 0$  by an amount  $\epsilon_0$ , which can be sufficient for this state to pass the limit  $E = 0$  as  $l_\perp$  decreases further. This new confined bound-state  $E'_B$  satisfies Eq.(1) with  $k^2$  replaced by  $2\mu E'_B / \hbar^2$ , i.e.,  $k_0 \equiv \pm i \sqrt{q_0^2 - 2\mu E'_B / \hbar^2}$ . Since the diverging term  $e^{ik_0 z}$  should be absent from Eq.(4a) and  $e^{ik_0 |z|}$  should decay,  $1/f_0^\pm$  must vanish at  $\text{Im}\{k_0\} > 0$ . From Eq.(13a), for  $a < 0$ , the virtual bound-state with energy  $E_B$  turns into a real one with energy  $E'_B$ , which starts at zero for  $a/d_\perp = 0$  and goes to a positive fraction of  $\epsilon_0$  as  $a/d_\perp \rightarrow -\infty$ . This bound-state exists only under confinement and its experimental measurement is reported in [15]. For  $a > 0$ , one obtains  $E'_B \rightarrow E_B$



for  $d_\perp \rightarrow \infty$ , as expected. For  $a \rightarrow +\infty$  (or  $d_\perp \rightarrow 0$ ),  $E'_B$  tends to a positive fraction of  $\epsilon_0$ . It turns out that the CIR condition (at  $a/d_\perp = 1/C' = \sqrt{3/20} \approx 0.39$ ) occurs before  $E'_B$  reaches zero (at  $a/d_\perp \approx 0.82$ ). On the other hand, the CIR almost coincides with the condition  $E'_B + (\epsilon_1 - \epsilon_0) = \epsilon_0$  (at  $a/d_\perp \approx 0.35$ ). In Ref. [10], this last coincidence is exact, since  $E'_B + (\epsilon_1 - \epsilon_0)$  can be associated with a bound-state of the excited channels  $n \geq 1$  due to a special property of the harmonic oscillator. However, despite this coincidence, a general mechanism behind CIR needs further study, since  $E'_B + (\epsilon_1 - \epsilon_0)$  has no clear meaning yet beyond parabolic guides and zero-range pseudopotentials.

*Excited Channels.* At energies  $k^2 = q_{n_E}^2 + k_{n_E}^2 > q_0^2$ , the case is more complex. Keeping only the  $l = 0$  wave as before, the  $n$ -th scattering amplitude  $f_n^\pm$  is

$$f_n^\pm \approx f_{ng} \approx -\frac{\sum_m b_m N_m / N_n}{1 + \sigma_n + i \left[ -\frac{d_\perp^2}{2} (-k \cot \delta_0 - P_{00}) \right] k_n}, \quad (14)$$

where  $0 \leq m, n \leq n_E$ ,  $P_{00} = (q_{1+n_E}^2 - k^2)^{1/2}$  and in  $\sigma_n \equiv \sum_{m \neq n} N_m^2 k_n / N_n^2 k_m$ ,  $m = n$  is excluded. For the *single* incoming excited channel  $n_E$ , i.e.,  $b_n = \delta_{n,n_E}$ , the amplitude  $f_{n_E g}$  does have the form Eq.(12) at small  $k_{n_E}$ . Thus, CIR at *threshold energies*  $k \rightarrow q_{n_E}$  can occur when  $-\tan \delta_0 / k = d_\perp / C'$  as first indicated in Ref. [11] for parabolic confinement. In a more realistic situation of finite temperatures  $T$ , however, for a given energy each  $b_n$  has the same weight (depending on  $E/T$  and with random phases). Since  $f_{ng} = -b_n$  cannot be met for all  $n$  simultaneously, one expects no sharp resonance, with the transmission and reflection probabilities being distributed among all channels according to Eq.(10c).

*l-couplings.* In the single mode regime, Eq.(10a) is also an equation for  $t_l \equiv T_l / k_0$  without the singularity  $\gamma \sim k_0^{-1}$ . If then  $\sum_{l' \neq l} (2l' + 1) P_{ll'} t_{l'}$  on the r.h.s converges, one can neglect it compared to  $\alpha_l$  for  $k_0 \rightarrow 0$ , and  $t_l \approx \alpha_l / [i\gamma k_0 k - (2l + 1)k_0 P_{ll} - k_0 k \cot \delta_l]$  is well behaved. Thus, angular momentum *couplings* should be negligible for  $k_0 \rightarrow 0$  and the series Eq.(10b) of individual momenta  $l$  is dominated by  $l = 0$  since  $\delta_l \sim k^{2l+1} \sim 1/l_\perp^{2l+1}$  are small, justifying Eq.(13a). This does not apply straightforwardly to the excited channel case, whose approximation is based only on the smallness of  $\delta_l$ .

*Discussion.* Consider now the case  $U(\rho) = \mu \omega_\perp^2 \rho^2 / 2$  of harmonic confinement,  $\mu$  being the reduced mass. In Eq.(13b), the oscillator length  $a_\perp \equiv (\hbar / \mu \omega_\perp)^{1/2}$  should replace  $d_\perp \equiv l_\perp / N_0$  instead of  $l_\perp$ . This is due to tunneling, since  $|\varphi_n(\rho)|^2 \sim e^{-\rho^2/a_\perp^2}$  is small at  $\rho \approx l_\perp$  (as in the square-well case) only if  $l_\perp > a_\perp$ . Then  $\epsilon_1 - \epsilon_0 \equiv \hbar^2(q_1^2 - q_0^2)/2\mu = 2\hbar\omega_\perp$  and  $C' = d_\perp \sqrt{q_1^2 - q_0^2} = 2$ . The difference to  $C = 1.4603 \dots$  of Ref. [9] originates from the

continuum limit in Eq.(5a) and Eq.(6b). Indeed, from Eq.(9) of Ref. [9], the continuum approximation for  $C$  is  $C \equiv \lim_{s \rightarrow \infty} (\int_0^s ds' / \sqrt{s'} - \sum_{s'=1}^s 1/\sqrt{s'}) \approx \int_0^1 ds' / \sqrt{s'} = 2$ . In addition, this comparison reveals the nature of the “irregular” part  $1/z$  of  $\Psi(\mathbf{r})$  for the pseudopotential approximation (see Eq.(8) of Ref. [9] or the equivalent  $s$ -wave expansion in Eq.(9) of Ref. [6]). This is the singular part of the free-space Green’s function  $\gamma_+ G_1 + \gamma_- G_2$ , with  $\gamma_+ + \gamma_- = 1$ , and originates from the sum of the excited transverse levels. As a result, one expects certain details of the guide to be unimportant, except for the low lying levels which account for the terms  $\gamma$  and  $\Delta_c$  and the bound-state  $E'_B$ .

We have provided a general treatment of quantum scattering in confined geometries. For scattering by obstacles inside the guide, the treatment should be applicable to a variety of central force fields  $V(r)$  and confining potentials  $U(\rho)$ . For ultracold atomic collisions, non-parabolic guides can be considered with restrictions due to the center of mass. The 1D scattering amplitude is given in terms of the free-space phase shifts  $\delta_l$  and their couplings among each other. This covers the case of higher energies and a transversal multi-channel incident state. In the single mode regime, we have shown that the CIR is closely related to the behaviour of a confined bound state.

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